EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1454	548/517.ccls.	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2008/01/31 14:28
L2	819	lactor	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2008/01/31 14:28
L3	1876	lactol	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2008/01/31 14:28
L4	18	l1 and l3	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2008/01/31 14:28

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Uploading C:\Program Files\Stnexp\Queries\10563459-broad.str

L1       STRUCTURE UPLOADED


=> d his

     (FILE 'HOME' ENTERED AT 14:24:15 ON 30 JAN 2008)

     FILE 'REGISTRY' ENTERED AT 14:24:23 ON 30 JAN 2008
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L3      1795381 S NC4/ES
L4       731680 S OC5/ES
L5        14238 S L3 AND L4
L6            0 S L1 SAM SUB=L5
L7            1 S L1 SSS FULL SUB=L5

     FILE 'CAPLUS' ENTERED AT 14:25:12 ON 30 JAN 2008
L8            1 S L7

     FILE 'REGISTRY' ENTERED AT 14:25:29 ON 30 JAN 2008

=> d l1
L1 HAS NO ANSWERS
L1              STR
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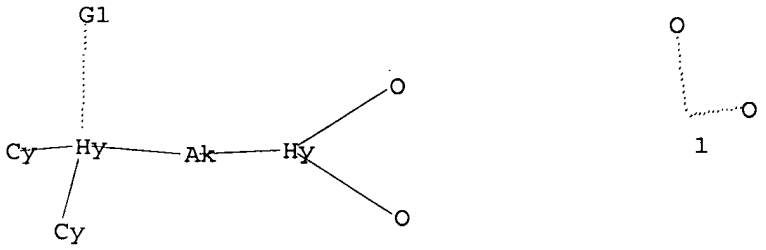


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G1 N,[@1]
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Structure attributes must be viewed using STN Express query preparation.

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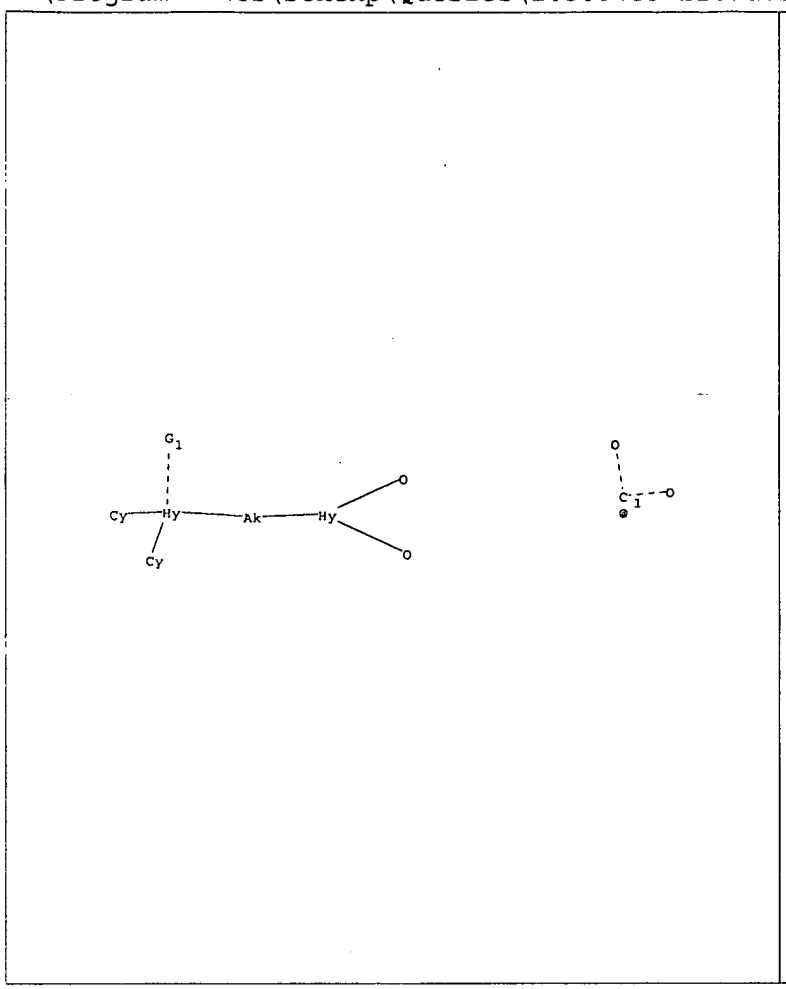

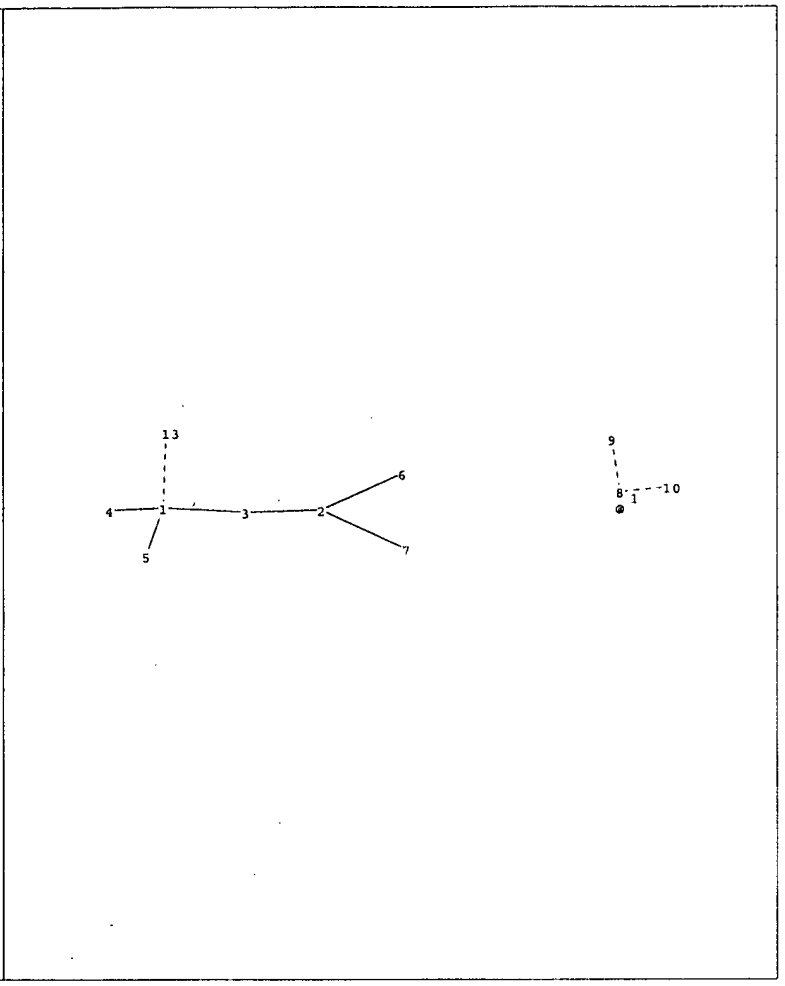

chain nodes :
1 2 3 4 5 6 7 8 9 10 13
chain bonds :
1-3 1-4 1-5 1-13 2-3 2-6 2-7 8-9 8-10
exact/norm bonds :
1-3 1-4 1-5 1-13 2-3 2-6 2-7 8-9 8-10

G1:N,[*1]

Connectivity :
3:2 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:CLASS 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
13:CLASS
Generic attributes :
1:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic
2:
Saturation : Saturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
3:
Saturation : Saturated

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Element Count :
    Node 1: Limited
        N,N1
        C,C4

    Node 2: Limited
        C,C5
        O,O1
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=> d l8 bib abs hitstr

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:120881 CAPLUS
DN 142:219082
TI Process for the preparation of statins, particularly atorvastatin, and useful intermediate compounds
IN Moody, David John; Wiffen, Jonathan William
PA Avecia Limited, UK
SO PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005012246	A1	20050210	WO 2004-GB3206	20040723
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	JP 2006528655	T	20061221	JP 2006-521652	20040723
	MX 2006PA00926	A	20060907	MX 2006-PA926	20060124
	NO 2006000903	A	20050126	NO 2006-903	20060224
	US 2007043221	A1	20070222	US 2006-563459	20060710
PRAI	GB 2003-17393	A	20030725		
	GB 2004-6760	A	20040326		
	WO 2004-GB3206	W	20040723		

OS CASREACT 142:219082; MARPAT 142:219082
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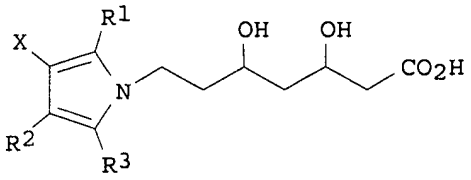

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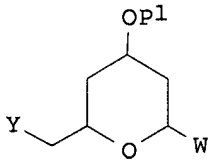

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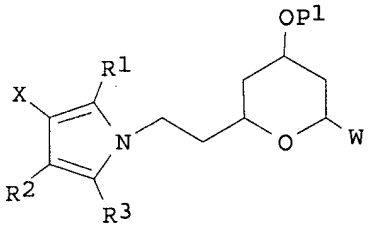

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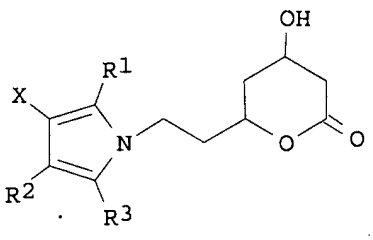


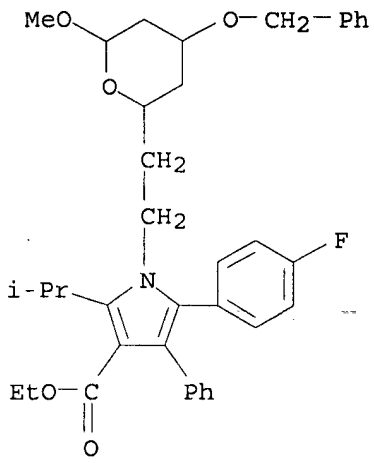
IV

AB There is provided a process for the preparation of a compound I [R1, R3 = H, hydrocarbyl; R2 = H, substituent; X = H, substituent] or salts thereof, which comprises: (a) cyanating pyran II [Y = halo (preferably Cl or Br); P1 = H, protecting group; W = :O or OP2; P2 = H, protecting group] to give pyran II (Y = CN); (b) reducing pyran II (Y = CN) to give amine pyran II (Y = CH2NH2); (c) coupling II (Y = CH2NH2) with dicarbonyl compound, R1COCHXCHR2COR3 to give pyranol III; (d) when W = OP2, deprotecting and then oxidizing III to give pyranone IV; and (e) subjecting III [W = O] or IV to ring-opening, and removal of any remaining protecting groups, to give pyrrole I. Thus, lipitor, the calcium salt of atorvastatin [I; R1 = CHMe2, R2 = Ph, R3 = C6H4F-4, X = CONHPh], was prepared from 6-(chloromethyl)tetrahydropyran-2,4-diol via methanolysis to the methylacetal, O-benzylation with PhCH2Br in THF containing NaH, cyanation with KCN in DMSO, reduction with borane-THF complex, cyclocondesantion with 4-FC6H4COCHPhCH(COCHMe2)CO2Et in THF containing MeCO2H, hydrogenolysis in MeOh containing catalytic Pd/C, hydrolysis with HCl in aqueous MeOH to the lipitor lactone, Dess-Martin oxidation to the lipitor lactone, and saponification with Ca(OH)2.

IT 840528-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of, with aniline; preparation of statins, particularly
atorvastatin, and useful intermediates)

RN 840528-11-2 CAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 5-(4-fluorophenyl)-2-(1-methylethyl)-4-phenyl-1-[2-[tetrahydro-6-methoxy-4-(phenylmethoxy)-2H-pyran-2-yl]ethyl]-, ethyl ester (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L1      STRUCTURE UPLOADED

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L10     STRUCTURE UPLOADED
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L3           40 S L1 SSS FULL

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L4           96 S L3

     FILE 'REGISTRY' ENTERED AT 10:10:31 ON 31 JAN 2008

     FILE 'STNGUIDE' ENTERED AT 10:11:14 ON 31 JAN 2008

     FILE 'REGISTRY' ENTERED AT 10:13:14 ON 31 JAN 2008
L5              SCREEN 1842
L6              SCREEN 1843
L7            2 S L1 AND L5 NOT L6 SAM
L8           28 S L1 AND L5 NOT L6 SSS FULL

     FILE 'CAPLUS' ENTERED AT 10:13:47 ON 31 JAN 2008
L9           92 S L8

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     FILE 'STNGUIDE' ENTERED AT 10:14:28 ON 31 JAN 2008

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L12           5 S L10 SSS FULL SUB=L8

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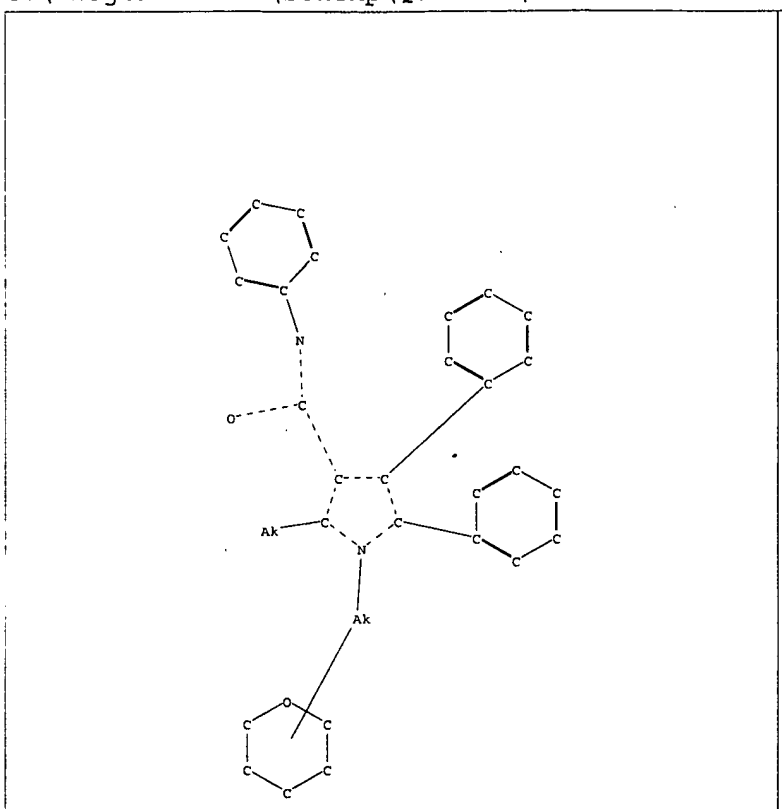

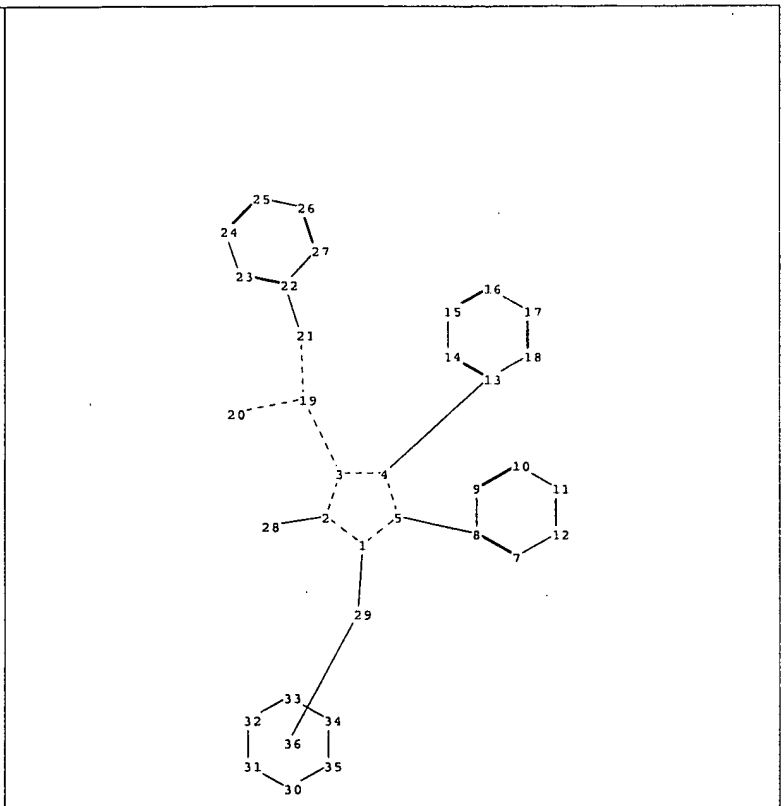

chain nodes :
19 20 21 28 29
ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 22 23 24 25 26 27 30
31 32 33 34 35
chain bonds :
1-29 2-28 3-19 4-13 5-8 19-20 19-21 21-22
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16
16-17 17-18 22-23 22-27 23-24 24-25 25-26 26-27 30-31 30-35 31-32 32-33
33-34 34-35
exact/norm bonds :
1-2 1-5 1-29 2-3 2-28 3-4 3-19 4-5 4-13 5-8 19-20 19-21 21-22 30-31 30-35
31-32 32-33 33-34 34-35
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18 22-23
22-27 23-24 24-25 25-26 26-27
isolated ring systems :
containing 1 : 7 : 13 : 22 : 30 :

Match level :
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12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS
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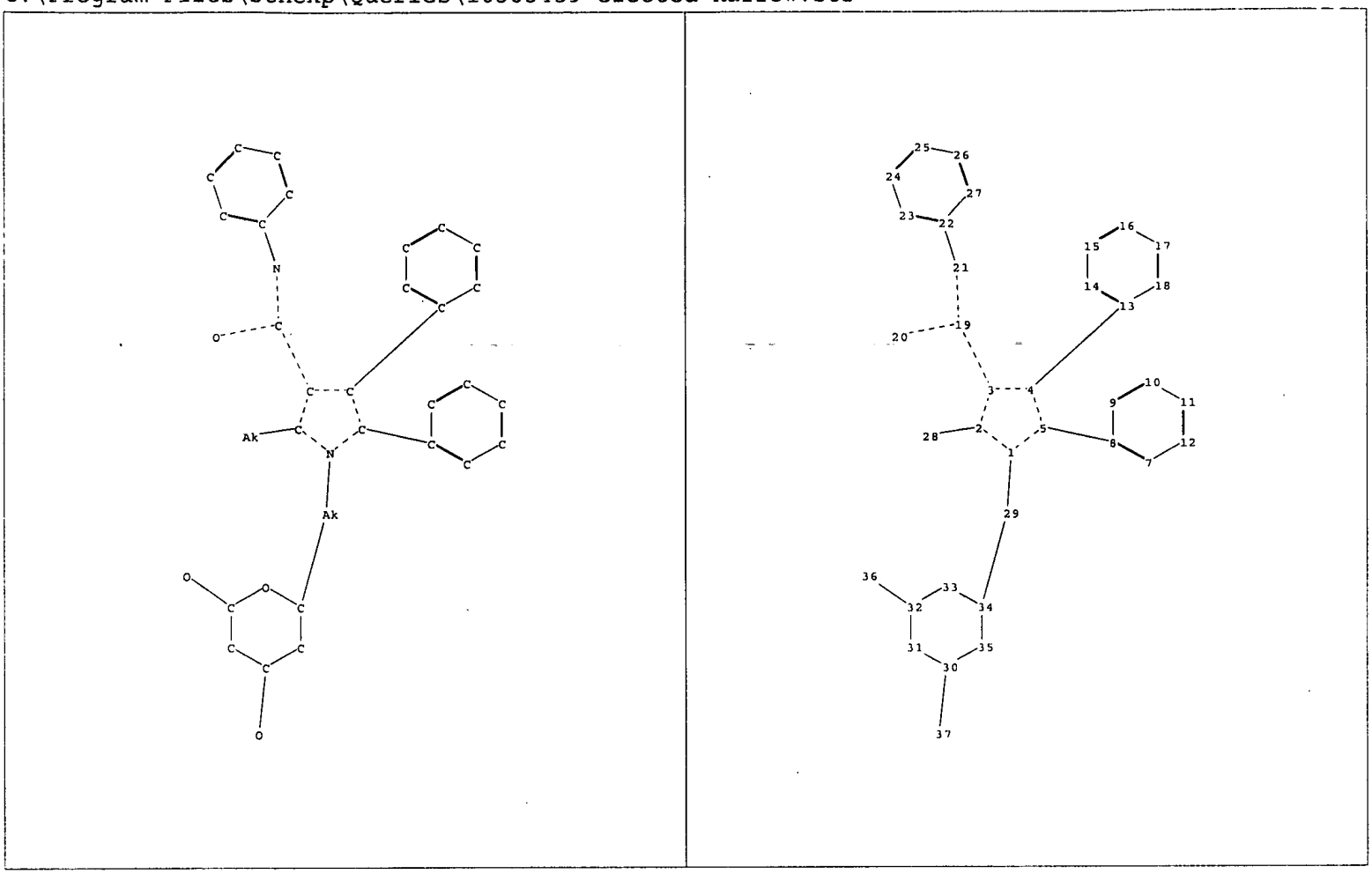

chain nodes :
19 20 21 28 29 36 37
ring nodes :
1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 22 23 24 25 26 27 30
31 32 33 34 35
chain bonds :
1-29 2-28 3-19 4-13 5-8 19-20 19-21 21-22 29-34 30-37 32-36
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16
16-17 17-18 22-23 22-27 23-24 24-25 25-26 26-27 30-31 30-35 31-32 32-33
33-34 34-35
exact/norm bonds :
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30-35 30-37 31-32 32-33 32-36 33-34 34-35
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18 22-23
22-27 23-24 24-25 25-26 26-27
isolated ring systems :
containing 1 : 7 : 13 : 22 : 30 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:CLASS 37:CLASS

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L13  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2007:1052509  CAPLUS
DN   147:385764
TI   Process for preparing C7 intermediates and their use in the preparation of
     N-substituted pyrrole derivatives
IN   Korostylev, Andrei; Tararov, Vitali; Boerner, Armin; Koenig, Gerd; Bobal,
     Pavel; Frantisek, Jaroslav; Stohandl, Jiri; Denike, Kane; Jeker, Nicolas
PA   Ratiopharm GmbH, Germany
SO   Eur. Pat. Appl., 56pp.
     CODEN: EPXXDW
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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           BA, HR, MK, YU
     WO 2007107276         A2    20070927    WO 2007-EP2245          20070314
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            KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN,
            MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,
            RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
        RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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            BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
            GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
            BY, KG, KZ, MD, RU, TJ, TM
PRAI EP 2006-5510          A     20060317
OS   MARPAT 147:385764
AB   The present invention relates to a process for preparing C7 intermediates and
     their use in the preparation of pyrrole derivs. of a class that is effective at
     inhibiting the biosynthesis of cholesterol in humans, and more
     particularly to improved synthetic methods for preparing 3,5-dihydroxy-7-
     pyrrol-1-ylheptanoic acids.  Thus, Et 5,5-dimethoxy-3-oxopentanoate was
     hydrogenated with Ru((R)-BINAP)Cl2 in MeOH to give (R)-Et
     5,5-dimethoxy-3-hydroxypentanoate with 97.8% ee.
RE.CNT  5     THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13  ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2005:120881  CAPLUS
DN   142:219082
TI   Process for the preparation of statins, particularly atorvastatin, and
     useful intermediate compounds
IN   Moody, David John; Wiffen, Jonathan William
PA   Avecia Limited, UK
SO   PCT Int. Appl., 22 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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SN, TD, TG

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OS CASREACT 142:219082; MARPAT 142:219082

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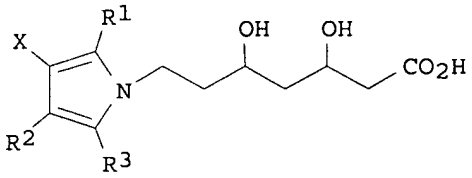

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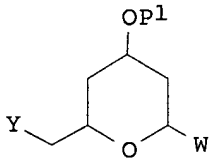

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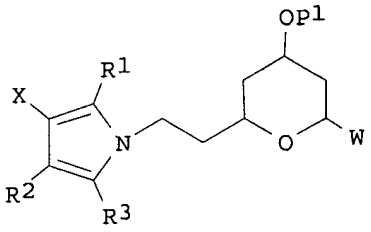

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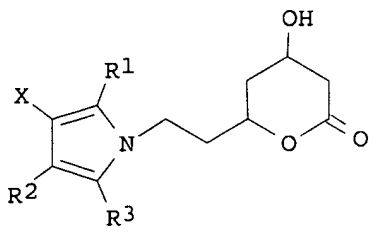

IV

AB There is provided a process for the preparation of a compound I [R1, R3 = H, hydrocarbyl; R2 = H, substituent; X = H, substituent] or salts thereof, which comprises: (a) cyanating pyran II [Y = halo (preferably Cl or Br); P1 = H, protecting group; W = :O or OP2; P2 = H, protecting group] to give pyran II (Y = CN); (b) reducing pyran II (Y = CN) to give amine pyran II (Y = CH2NH2); (c) coupling II (Y = CH2NH2) with dicarbonyl compound, R1COCHXCHR2COR3 to give pyranol III; (d) when W = OP2, deprotecting and then oxidizing III to give pyranone IV; and (e) subjecting III [W = O] or IV to ring-opening, and removal of any remaining protecting groups, to give pyrrole I. Thus, lipitor, the calcium salt of atorvastatin [I; R1 =

CHMe2, R2 = Ph, R3 = C6H4F-4, X = CONHPh], was prepared from 6-(chloromethyl)tetrahydropyran-2,4-diol via methanolysis to the methylacetal, O-benzylation with PhCH2Br in THF containing NaH, cyanation with KCN in DMSO, reduction with borane-THF complex, cyclocondesantion with 4-FC6H4COCHPhCH(COCHMe2)CO2Et in THF containing MeCO2H, hydrogenolysis in MeOh containing catalytic Pd/C, hydrolysis with HCl in aqueous MeOH to the lipitor lactone, Dess-Martin oxidation to the lipitor lactone, and saponification with Ca(OH)2.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4       STRUCTURE UPLOADED

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Uploading C:\Program Files\Stnexp\Queries\10563459-elected.str

L5       STRUCTURE UPLOADED
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L5                STRUCTURE UPLOADED
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L7         483280 S L4 SSS FULL
L8              2 S L5
L9             40 S L5 SSS FULL

     FILE 'CAPLUS' ENTERED AT 12:24:02 ON 31 JAN 2008

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     FILE 'REGISTRY' ENTERED AT 12:24:43 ON 31 JAN 2008

     FILE 'REGISTRY' ENTERED AT 12:25:08 ON 31 JAN 2008

     FILE 'REGISTRY' ENTERED AT 12:26:10 ON 31 JAN 2008
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L11               SCREEN 1839
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L13         64431 S L4 AND L10 NOT L11 SSS FULL

     FILE 'CAPLUS' ENTERED AT 12:26:59 ON 31 JAN 2008

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L15          96 L9

=> s l14 and l15
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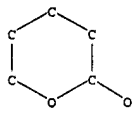

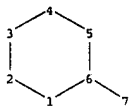

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ring nodes :
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chain bonds :
6-7
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
6-7
exact bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS

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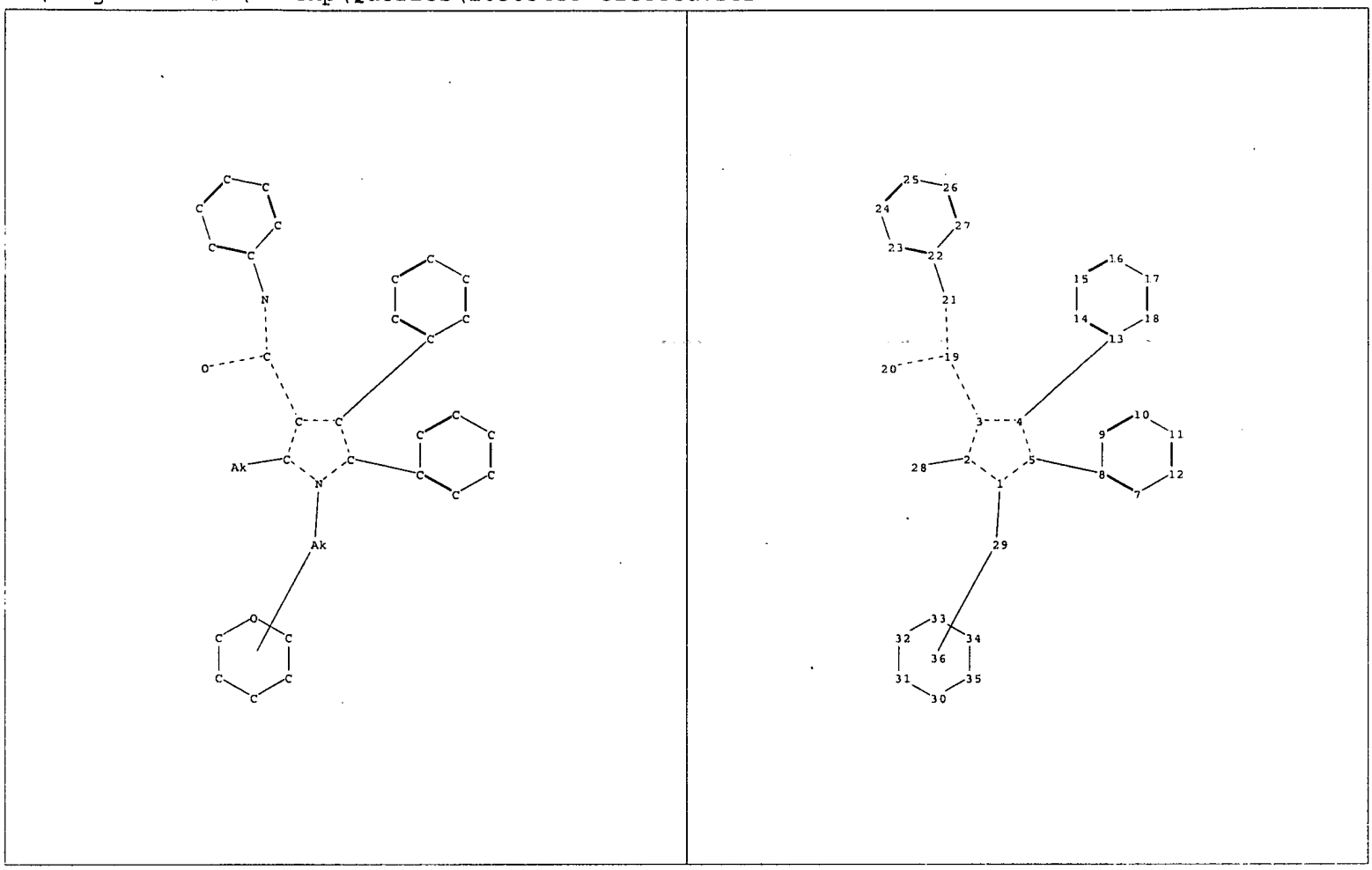

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ring nodes :
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31 32 33 34 35
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ring bonds :
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16-17 17-18 22-23 22-27 23-24 24-25 25-26 26-27 30-31 30-35 31-32 32-33
33-34 34-35
exact/norm bonds :
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31-32 32-33 33-34 34-35
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22-27 23-24 24-25 25-26 26-27
isolated ring systems :
containing 1 : 7 : 13 : 22 : 30 :

Match level :
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12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom

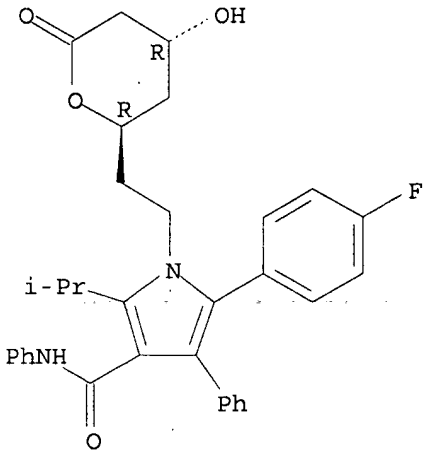
L16 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:999457 CAPLUS
DN 147:308266
TI Stable non-crystalline oral pharmaceutical formulation comprising HMG-CoA reductase inhibitor such as atorvastatin
IN Palepu, Nageshwara; Kordikowski, Andreas; Zhang, Jiang; Duddu, Sarma; Lechuga, David; Kuo, Mei Chang
PA Scidose, LLC, USA
SO PCT Int. Appl., 103pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007100614	A2	20070907	WO 2007-US4629	20070220

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

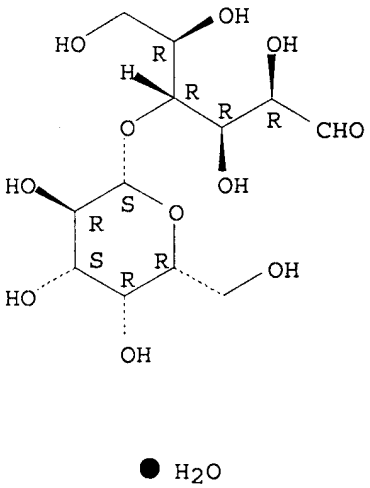
PRAI US 2006-776525P P 20060224
OS MARPAT 147:308266
AB One or more embodiments of the present invention relate to a formulation comprising an HMG-CoA reductase inhibitor, to co-formulations of HMG-CoA reductase inhibitors with excipients, to methods for preparing the formulations, pharmaceutical compns. comprising the formulations and to their use in medical treatment. Also provided are stable oral pharmaceutical formulations comprising HMG-CoA reductase inhibitors such as atorvastatin, an associated methods for their preparation and use of (administering) the stable oral pharmaceutical formulations and co-formulations. The formulations which result in desired, especially improved or enhanced, solubility or dissoln. characteristics, resulting in desired, especially improved or enhanced, bioavailability and/or pharmacokinetics. Thus, coformulation of atorvastatin calcium with an excipient, hydroxypropylcellulose, was prepared by mixing 80 g hydroxypropyl cellulose and 720 g atorvastatin calcium in methanol, with solvent removal using CO2 as antisolvent.
IT 125995-03-1, Atorvastatin lactone
RL: RCT (Reactant); RACT (Reactant or reagent)
(stable non-crystalline oral pharmaceutical formulation comprising HMG-CoA reductase inhibitor such as atorvastatin)
RN 125995-03-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 64044-51-5, Pharmatose 200M
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(stable non-crystalline oral pharmaceutical formulation comprising HMG-CoA reductase inhibitor such as atorvastatin)
RN 64044-51-5 CAPLUS
CN D-Glucose, 4-O-β-D-galactopyranosyl-, hydrate (1:1) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



● H_2O

L16 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:120881 CAPLUS
DN 142:219082
TI Process for the preparation of statins, particularly atorvastatin, and useful intermediate compounds
IN Moody, David John; Wiffen, Jonathan William
PA Avecia Limited, UK
SO PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005012246	A1	20050210	WO 2004-GB3206	20040723

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

AU	2004261468	A1	20050210	AU 2004-261468	20040723
CA	2530163	A1	20050210	CA 2004-2530163	20040723
EP	1648866	A1	20060426	EP 2004-767938	20040723
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CN	1829688	A	20060906	CN 2004-80021382	20040723
BR	2004012786	A	20060926	BR 2004-12786	20040723
JP	2006528655	T	20061221	JP 2006-521652	20040723
MX	2006PA00926	A	20060907	MX 2006-PA926	20060124
NO	2006000903	A	20050126	NO 2006-903	20060224
US	2007043221	A1	20070222	US 2006-563459	20060710
PRAI GB	2003-17393	A	20030725		
GB	2004-6760	A	20040326		
WO	2004-GB3206	W	20040723		

OS CASREACT 142:219082; MARPAT 142:219082

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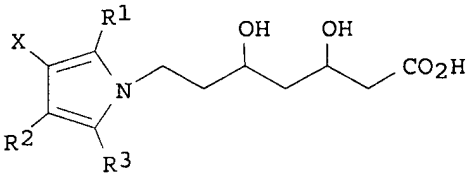

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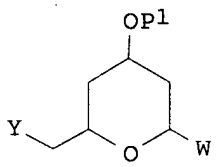

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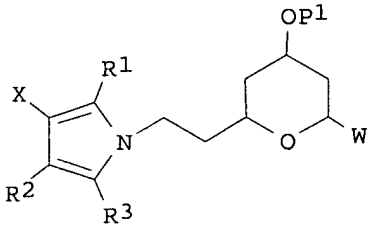

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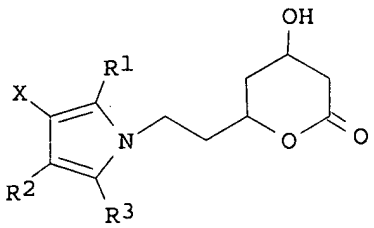


IV

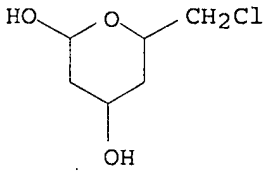
AB There is provided a process for the preparation of a compound I [R1, R3 = H, hydrocarbyl; R2 = H, substituent; X = H, substituent] or salts thereof, which comprises: (a) cyanating pyran II [Y = halo (preferably Cl or Br); P1 = H, protecting group; W = :O or OP2; P2 = H, protecting group] to give pyran II (Y = CN); (b) reducing pyran II (Y = CN) to give amine pyran II (Y = CH2NH2); (c) coupling II (Y = CH2NH2) with dicarbonyl compound, R1COCHXCHR2COR3 to give pyranol III; (d) when W = OP2, deprotecting and then oxidizing III to give pyranone IV; and (e) subjecting III [W = O] or IV to ring-opening, and removal of any remaining protecting groups, to give pyrrole I. Thus, lipitor, the calcium salt of atorvastatin [I; R1 = CHMe2, R2 = Ph, R3 = C6H4F-4, X = CONHPh], was prepared from 6-(chloromethyl)tetrahydropyran-2,4-diol via methanolysis to the

methylacetal, O-benzylation with PhCH2Br in THF containing NaH, cyanation with KCN in DMSO, reduction with borane-THF complex, cyclocondesantion with 4-FC6H4COCHPhCH(COCHMe2)CO2Et in THF containing MeCO2H, hydrogenolysis in MeOh containing catalytic Pd/C, hydrolysis with HCl in aqueous MeOH to the lipitor lactone, Dess-Martin oxidation to the lipitor lactone, and saponification with Ca(OH)2.

IT 159223-55-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(methanolysis of; preparation of statins, particularly atorvastatin, and useful intermediates)

RN 159223-55-9 CAPLUS

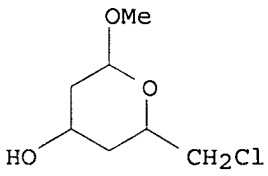
CN 2H-Pyran-2,4-diol, 6-(chloromethyl)tetrahydro- (CA INDEX NAME)



IT 840528-03-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-benzylation of; preparation of statins, particularly atorvastatin, and useful intermediates)

RN 840528-03-2 CAPLUS

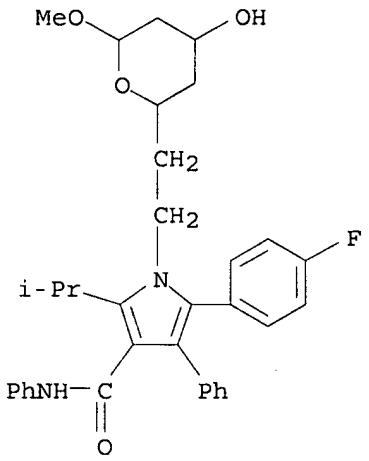
CN 2H-Pyran-4-ol, 2-(chloromethyl)tetrahydro-6-methoxy- (CA INDEX NAME)



IT 840528-15-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acid hydrolysis of; preparation of statins, particularly atorvastatin, and useful intermediates)

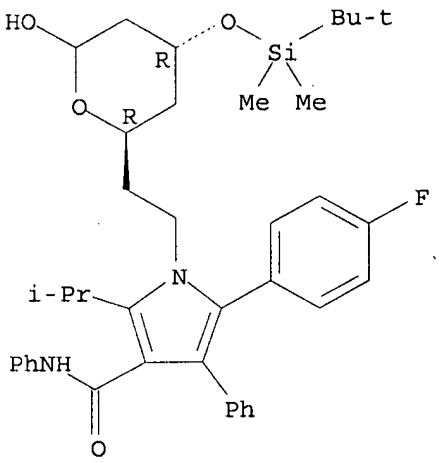
RN 840528-15-6 CAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-(tetrahydro-4-hydroxy-6-methoxy-2H-pyran-2-yl)ethyl]- (CA INDEX NAME)

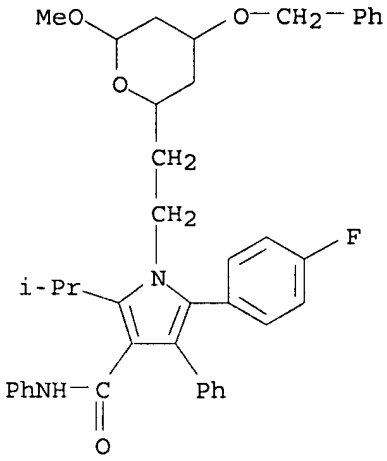


IT 840528-23-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of; preparation of statins, particularly atorvastatin, and useful intermediates)
RN 840528-23-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-[2-[(2R,4R)-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]tetrahydro-6-hydroxy-2H-pyran-2-yl]ethyl]-5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl- (CA INDEX NAME)

Absolute stereochemistry.

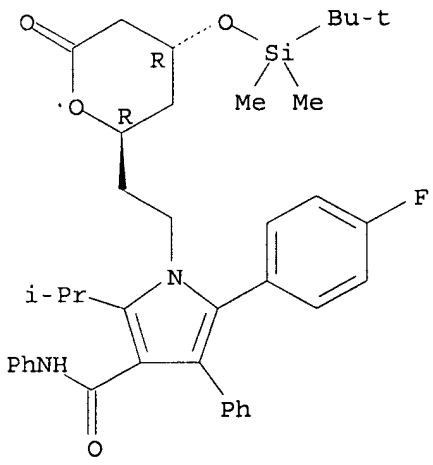


IT 840528-13-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolytic debenzylation of; preparation of statins, particularly atorvastatin, and useful intermediates)
RN 840528-13-4 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-[tetrahydro-6-methoxy-4-(phenylmethoxy)-2H-pyran-2-yl]ethyl]- (CA INDEX NAME)

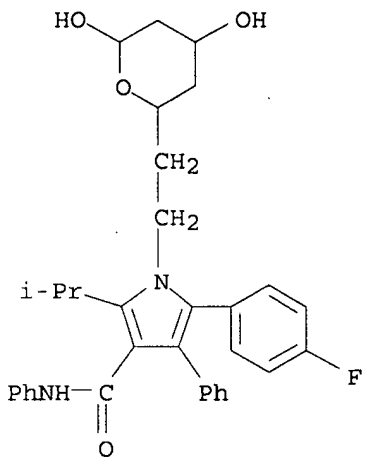


IT 842162-99-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of; preparation of statins, particularly atorvastatin, and
useful intermediates)
RN 842162-99-6 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-[2-[(2R,4R)-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]tetrahydro-6-oxo-2H-pyran-2-yl]ethyl]-5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl- (CA INDEX NAME)

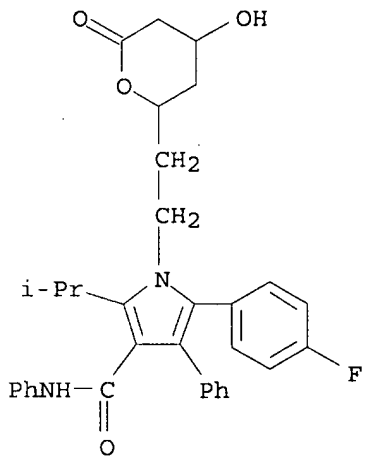
Absolute stereochemistry.



IT 840528-17-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and regioselective oxidation of, with Dess-Martin reagent; preparation
of statins, particularly atorvastatin, and useful intermediates)
RN 840528-17-8 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-(tetrahydro-4,6-dihydroxy-2H-pyran-2-yl)ethyl]- (CA INDEX NAME)

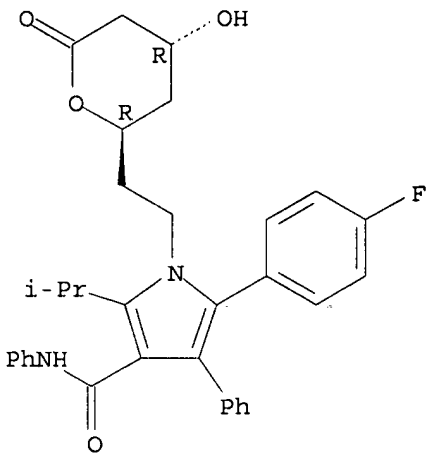


IT 160449-60-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and silylation or saponification of, with calcium hydroxide; preparation of
statins, particularly atorvastatin, and useful intermediates)
RN 160449-60-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-(tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl)ethyl]- (CA INDEX NAME)



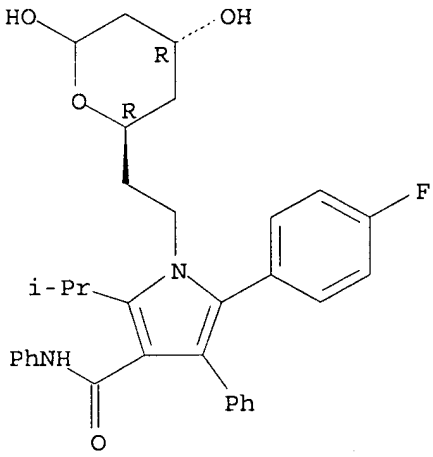
IT 125995-03-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of statins, particularly atorvastatin, and useful intermediates)
RN 125995-03-1 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 842163-03-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of statins, particularly atorvastatin, and useful intermediates)
RN 842163-03-5 CAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-[(2R,4R)-tetrahydro-4,6-dihydroxy-2H-pyran-2-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:1080531 CAPLUS
DN 142:62698
TI Pharmaceutical compositions of atorvastatin
IN Luner, Paul E.; Waterman, Kenneth Craig
PA Warner-Lambert LLC, USA
SO U.S. Pat. Appl. Publ., 17 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004253305	A1	20041216	US 2004-828398	20040420

PI US 2005032880 A1 20050210 US 2004-828488 20040420
CA 2465640 A1 20041212 CA 2004-2465640 20040429
CA 2465693 A1 20041212 CA 2004-2465693 20040429
AU 2004246867 A1 20041223 AU 2004-246867 20040601
WO 2004110406 A1 20041223 WO 2004-IB1859 20040601
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EP 1635788 A1 20060322 EP 2004-735617 20040601
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BR 2004011313 A 20060711 BR 2004-11313 20040601
BR 2004011354 A 20060711 BR 2004-11354 20040601
CN 1805732 A 20060719 CN 2004-80016386 20040601
JP 2006527259 T 20061130 JP 2006-516511 20040601
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IN 2005DN04772 A 20071207 IN 2005-DN4772 20051019
MX 2005PA12954 A 20060213 MX 2005-PA12954 20051130
MX 2005PA12955 A 20060213 MX 2005-PA12955 20051130
KR 760112 B1 20070918 KR 2005-723718 20051209
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PRAI US 2003-477916P P 20030612
US 2003-477917P P 20030612
WO 2004-IB1859 W 20040601
WO 2004-IB1879 W 20040601

AB The invention describes a dry-granulated pharmaceutical composition comprising atorvastatin or a pharmaceutically acceptable salt thereof, as well as a dry-granulated pharmaceutical composition comprising atorvastatin or a pharmaceutically acceptable salt thereof in combination with at least one other active drug, methods for preparing said compns., kits for containing such compns., and a method of treating hypercholesterolemia and/or hyperlipidemia, osteoporosis, benign prostatic hyperplasia (BPH), and Alzheimer's disease using a therapeutically effective amount of the pharmaceutical composition For example, atorvastatin tablets were prepared by a wet granulation of a composition containing 2.59 g of spray dried amorphous atorvastatin, 78.00 g of microcryst. cellulose, 101.41 g of lactose, 6.00 g of croscarmellose sodium (Ac-Di-Sol), and 4.000 g of hydroxypropyl cellulose (Klucel EXF). To 175.0 g of the dried granules was added 5.469 g of Ac-Di-Sol followed by 1.822 g of magnesium stearate and the mixture was compressed to give .apprx.250 tablets. After storage of tablets for 4 wk

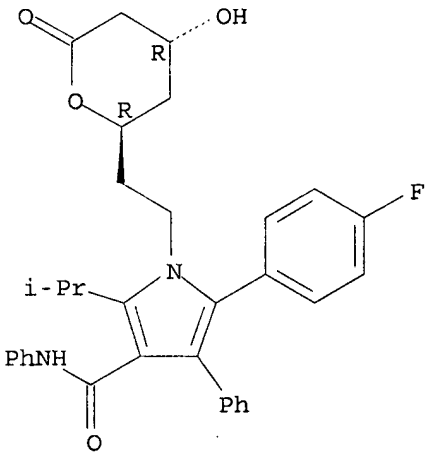
at 40° and 75% relative humidity, the level of atorvastatin lactone was 25.4%.

IT 125995-03-1, Atorvastatin lactone
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (preparation and stability of atorvastatin granulations, tablets and capsules)

RN 125995-03-1 CAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl]- (CA INDEX NAME)

Absolute stereochemistry.

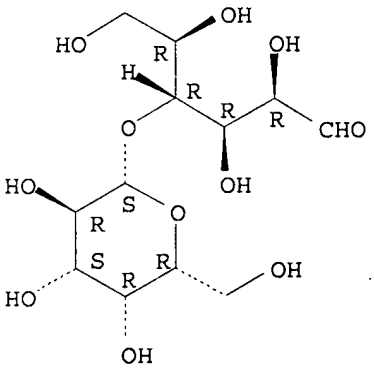


IT 63-42-3, Lactose
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (preparation and stability of atorvastatin granulations, tablets and capsules)

RN 63-42-3 CAPLUS

CN D-Glucose, 4-O-β-D-galactopyranosyl- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION

CA SUBSCRIBER PRICE -2.40 -3.15

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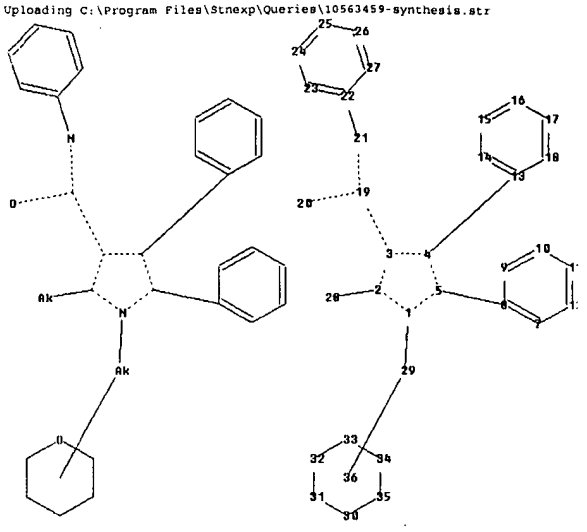

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ring nodes :
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30 31 32 33 34 35
chain bonds :
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ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
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32-33 33-34
34-35
exact/norm bonds :
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30-35 31-32 32-33 33-34 34-35
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18 22-23
22-27 23-24 24-25 25-26 26-27
isolated ring systems :
containing 1 : 7 : 13 : 22 : 30 :

Match level :
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12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:Atom 31:Atom
32:Atom 33:Atom
34:Atom 35:Atom 36:Atom
fragments assigned product role:
containing 1

L1 STRUCTURE UPLOADED

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100.0% DONE 24 VERIFIED 3 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 187 TO 773
PROJECTED ANSWERS: 1 TO 79

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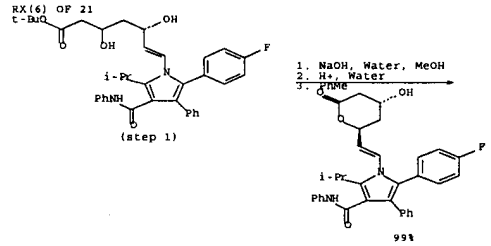
L3 ANSWER 1 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

RX(6) OF 21



(step 1)

1. NaOH, Water, MeOH
2. H+, Water
3. PhMe

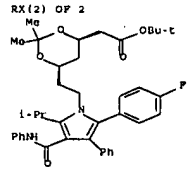
99%

REF: Mex. Pat. Appl., 2000PA12407, 17 Jan 2006

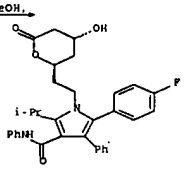
CON: STAGE(2) pH 3.8
STAGE(3) 6 hours, 90 deg C

L3 ANSWER 2 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 2



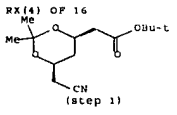
H2NOH-HCl, MeOH, Me2CO, water



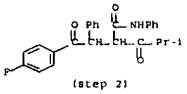
REF: PCT Int. Appl., 2007028412, 15 Mar 2007
CON: STAGE(1) room temperature -> 67 deg C, 1 hour, 67 deg C

L3 ANSWER 3 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 16



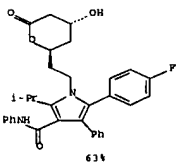
(step 1)



(step 2)

1. Ni, NH3, H2, Water, Me2CHOH
2. t-BuCO2H, THF, Hexane
3. HCl, Water, MeOH
4. NaOH, water, t-BuOMe
5. HCl, Water
6. PhMe

RX(4) OF 16

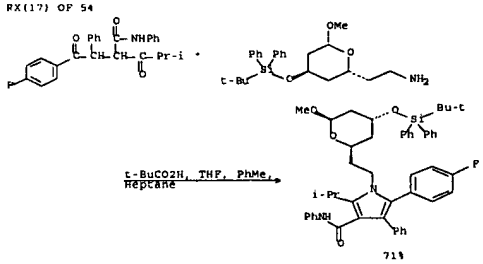


63%

REF: PCT Int. Appl., 2007029216, 15 Mar 2007
NOTE: wet sponge nickel catalyst was used in first stage
CON: STAGE(2) 96 hours, room temperature -> 75 deg C
STAGE(3) 10 deg C
STAGE(4) 10 deg C
STAGE(6) 4 hours, reflux

L3 ANSWER 4 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

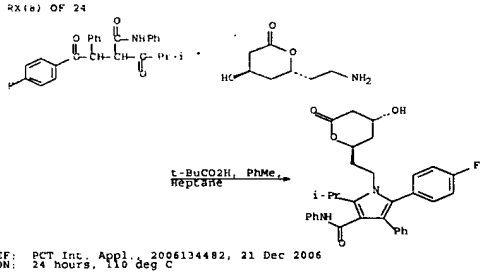
RX(17) OF 54



REF: European Journal of Organic Chemistry, (24), 5543-5550; 2006
CON: STAGE(1) 10 hours, reflux; cooled

L3 ANSWER 5 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

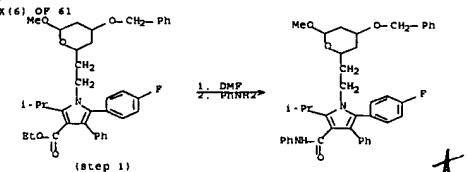
RX(8) OF 24



REF: PCT Int. Appl., 2006134482, 21 Dec 2006
CON: 24 hours, 110 deg C

L3 ANSWER 6 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

RX(6) OF 61

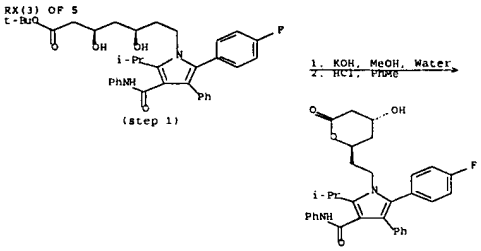


REF: PCT Int. Appl., 2005012246, 10 Feb 2005
CON: STAGE(2) 18 hours, 80 deg C

instant

L3 ANSWER 7 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 5



REF: PCT Int. Appl., 2004014896, 19 Feb 2004

L3 ANSWER 8 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

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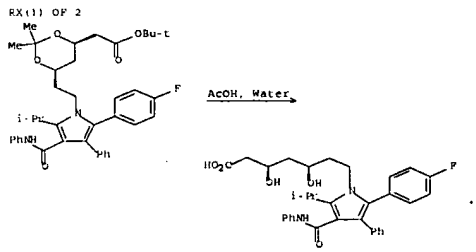

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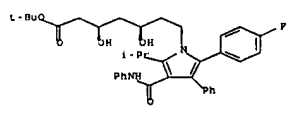

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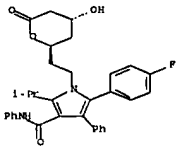

REF: PCT Int. Appl., 2002043667, 06 Jun 2002

L3 ANSWER 9 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

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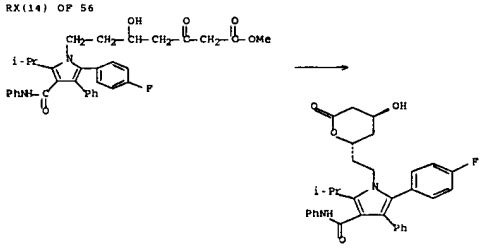

REF: Journal of Medicinal Chemistry, 34(1), 357-66; 1991

L3 ANSWER 10 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

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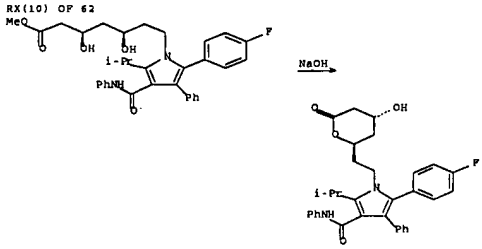

REF: PCT Int. Appl., 8907598, 24 Aug 1989

L3 ANSWER 11 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

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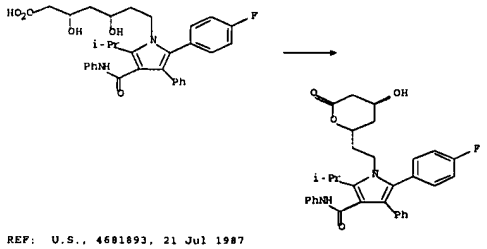

REF: U.S., 4681893, 21 Jul 1987

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